



# Aspects of Cool-Flame Supported Droplet Combustion in Microgravity

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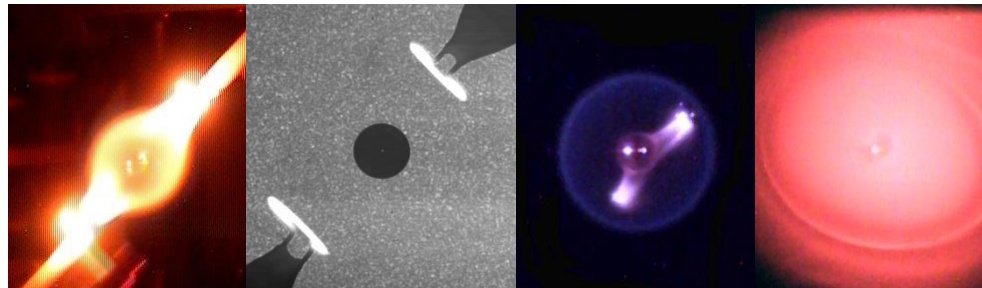
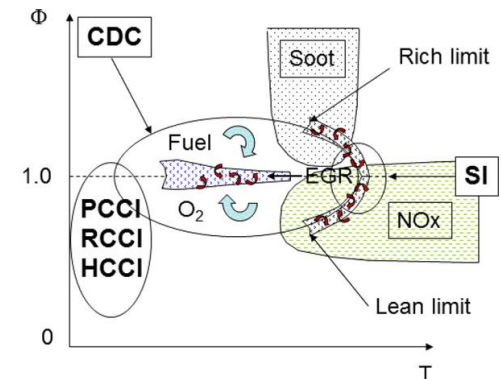
Forman A. Williams  
University of California, San Diego, La Jolla, CA



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Alexandria, VA U.S.A

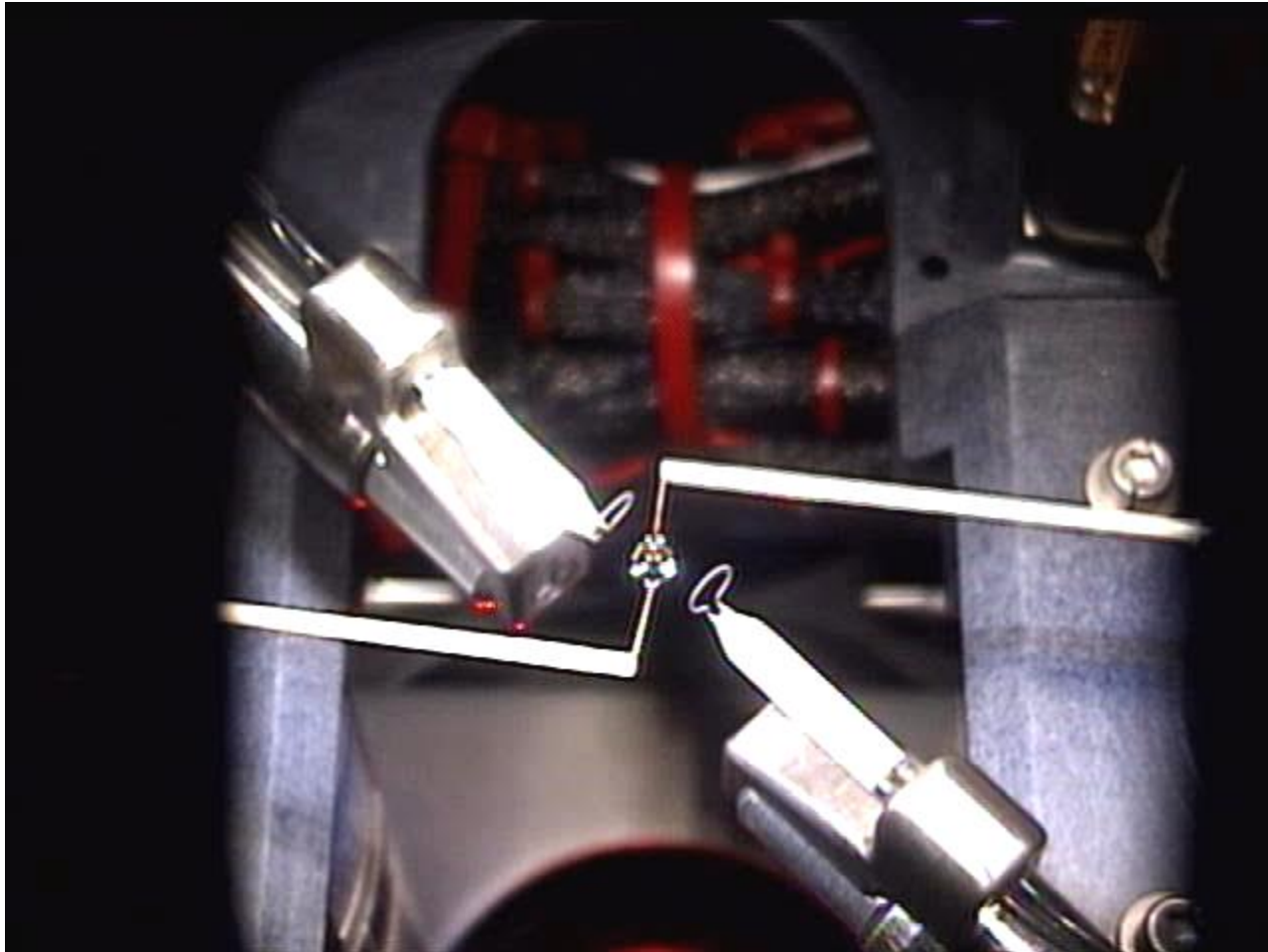
# Cool Flames

- Accidentally discovered by Sir Humphry Davy in 1810
- Historically cool flames are associated with premixed combustion leading to ignition of fuel/air mixtures. (commonly encountered in car-engine knock)
- More recently diffusion-controlled, quasi-steady cool flames supporting droplet combustion were discovered the FLEX team
- Cool-flame low-T chemistry is of importance in new engine designs, fuel reforming, etc.
- Important implications with regard to space craft fire safety



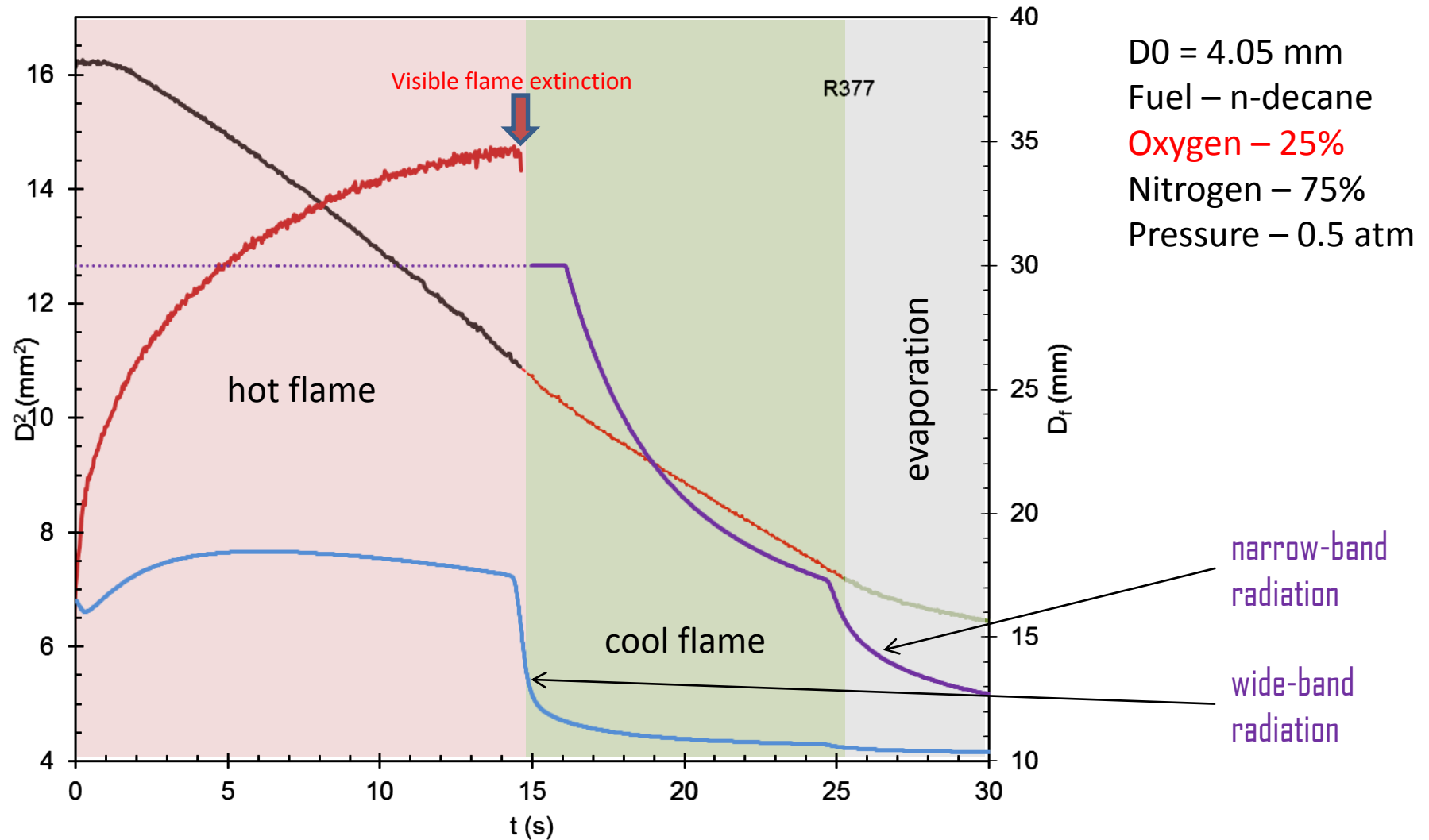
## Flame Extinguishment Experiments: FLEX

- Droplet combustion experiments being conducted onboard the International Space Station

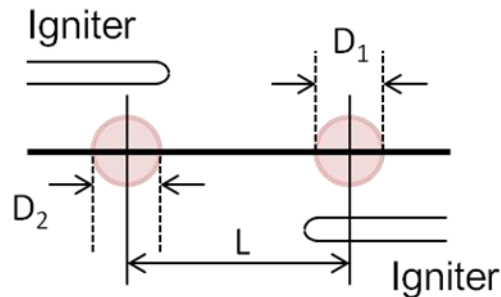
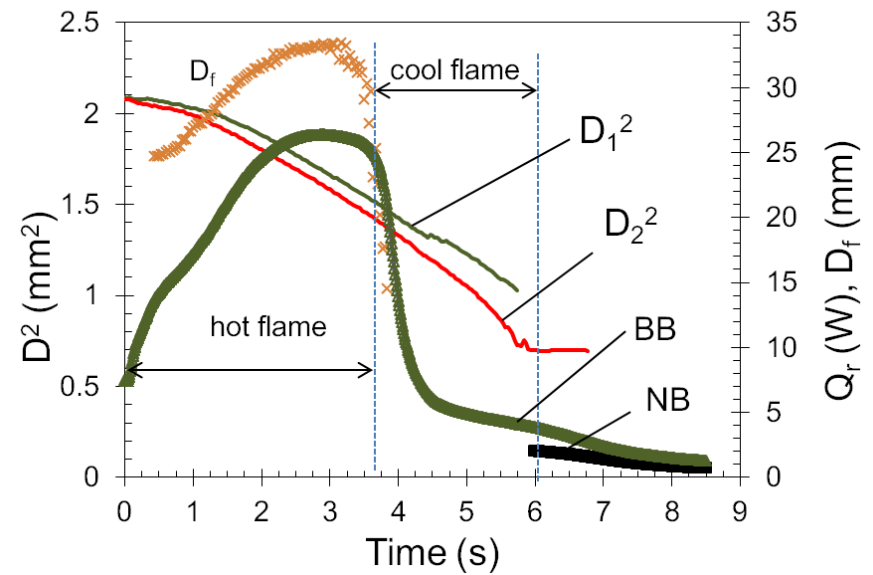
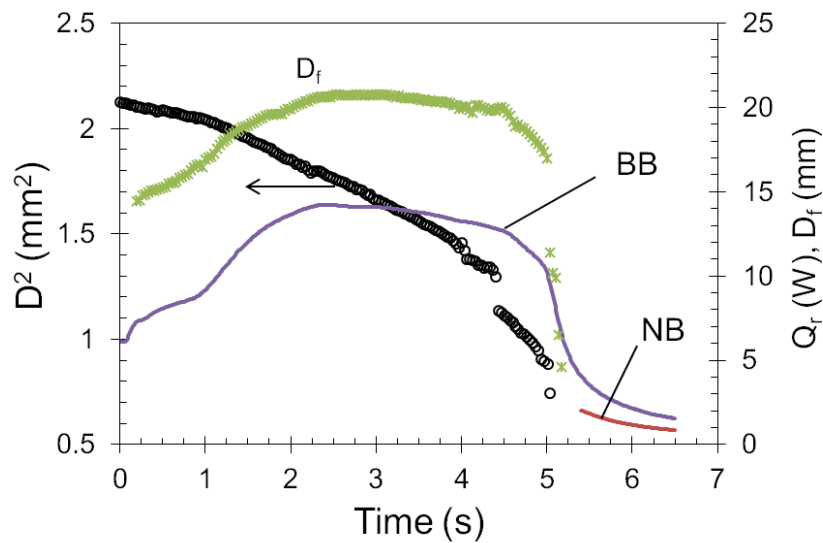


# FLEX Cool Flame – Pure Fuels

FLEX-377: N-Decane burning in  $O_2/N_2$  environment

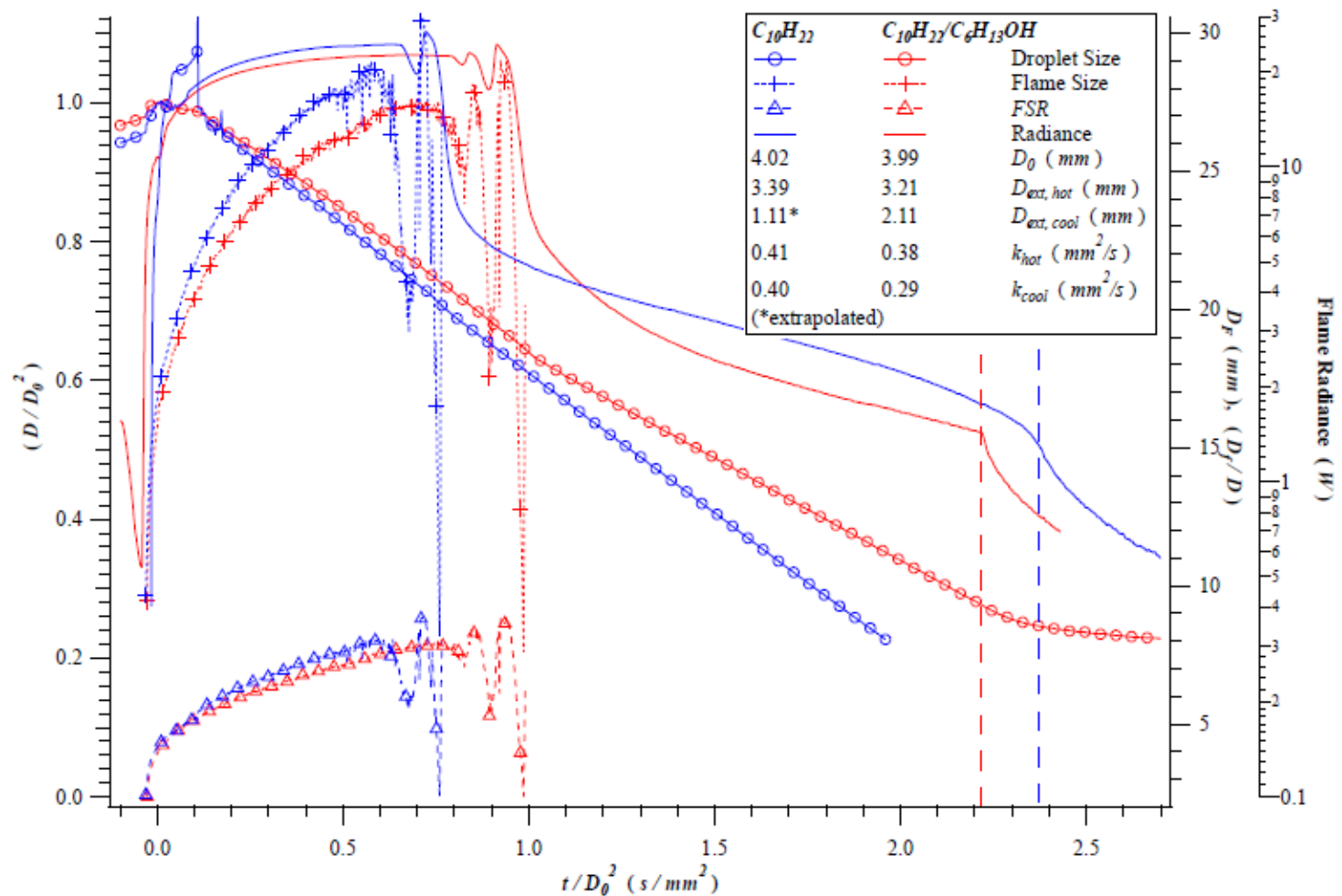


# FLEX Cool Flame – Binary Droplet Arrays



- N-decane droplets burning in 17-83%  $O_2$ - $N_2$  ambient at 1 atm
- Similar size droplets: Single droplets only hot flame – Binary droplets cool flame

# FLEX Cool Flame – Fuel Mixtures



- Decane/Hexanol droplet compared to pure Decane droplet – 1 atm in air
- Alcohol slows the CF burning rate and increases the extinction diameter

# Theoretical Models for Cool Flame Combustion

# Liñán's Diffusion Flame Regimes

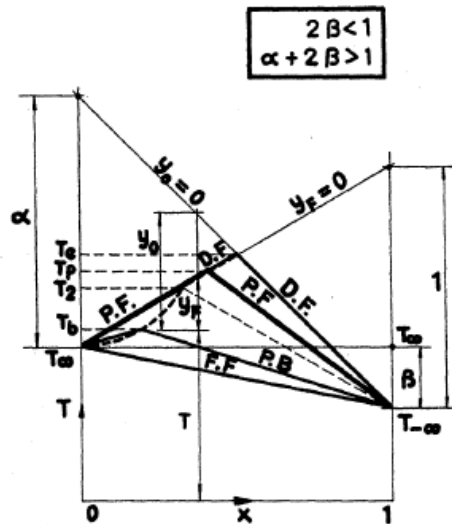
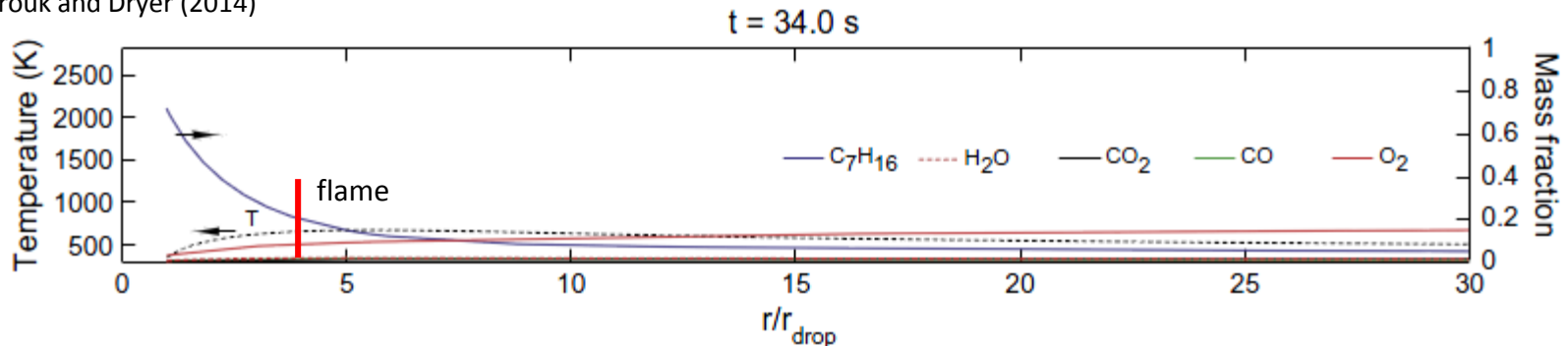


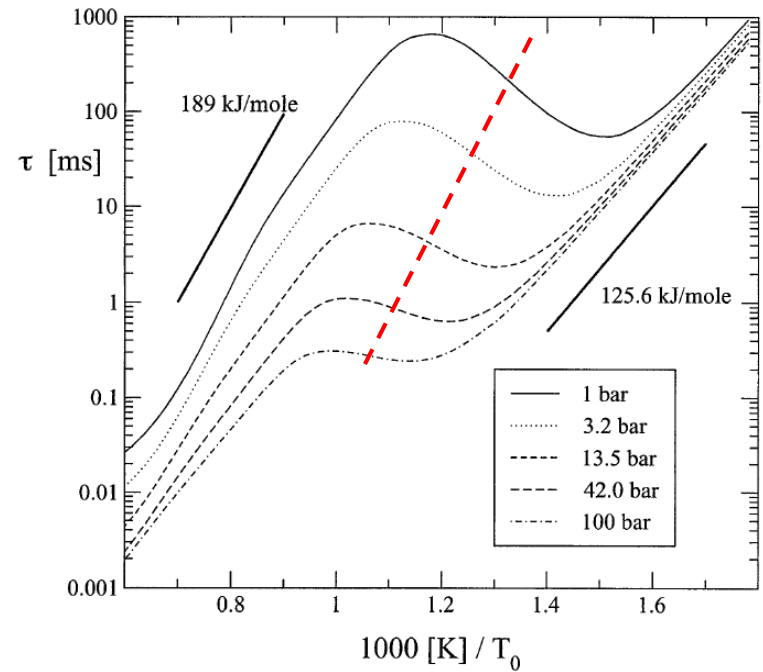
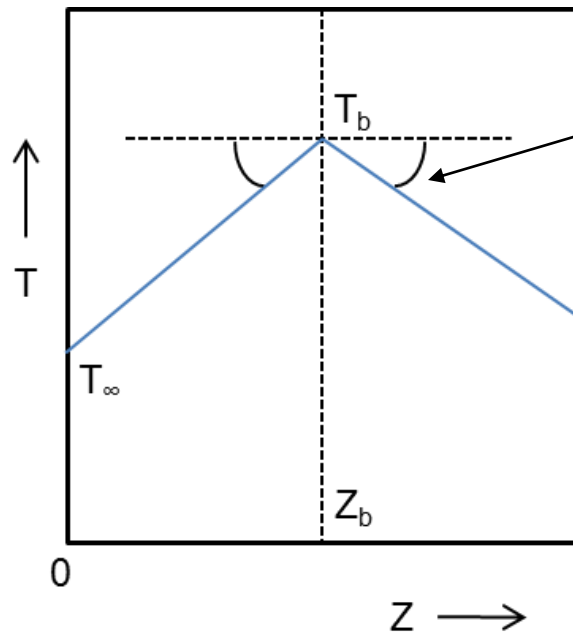
Fig. 2. Asymptotic temperature and concentration distributions for the frozen flow, partial burning (P.B.), premixed flame, and diffusion controlled regime for the case  $2\beta < 1$  and  $\alpha + 2\beta > 1$ , when the flame lies always in the lean side of the mixing layer.

- In the limit of large activation energies, Linan showed that structure of diffusion flames can be captured in terms of 4 regimes
  - Frozen-flow
  - **Partial-burning**
  - Premixed-flame
  - Near-equilibrium diffusion flame
- Since both fuel and oxygen leaks through the flame *partial-burning regime* is appropriate for cool-flame combustion of droplets

Farouk and Dryer (2014)



# Liñán's Partial Burning Regime



$$Z < Z_b : T = T_{\infty} + \frac{(T_b - T_{\infty})}{Z_b} Z,$$

$$Z > Z_b : T = T_1 + \frac{(T_b - T_1)}{(1 - Z_b)} (1 - Z),$$

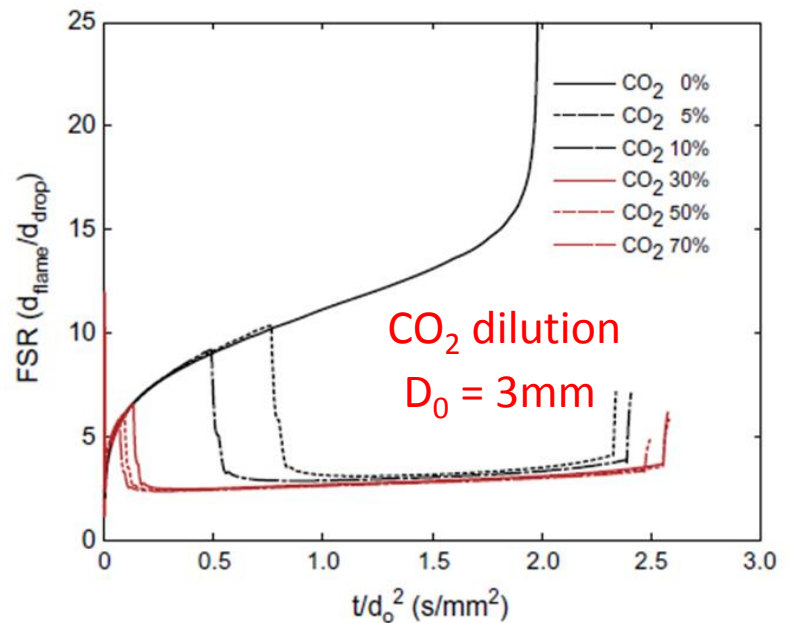
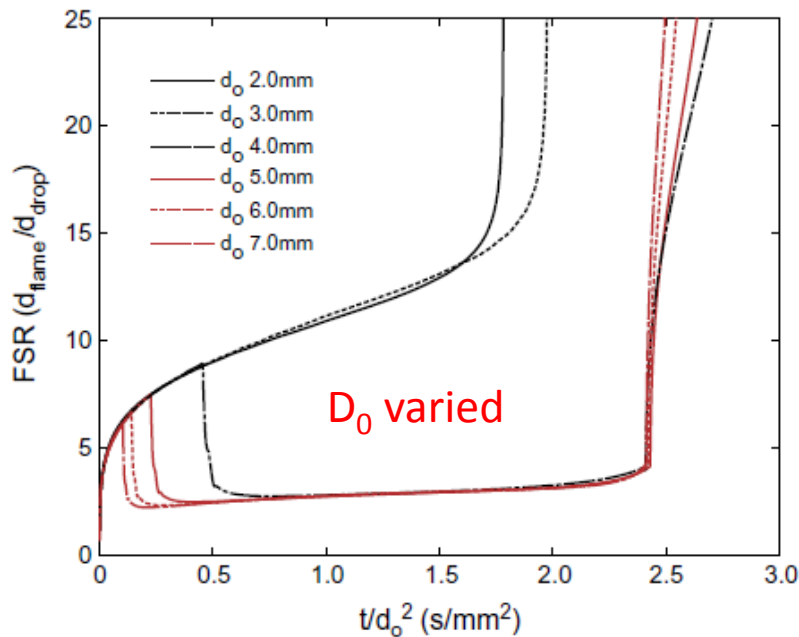
$$Z_b = \frac{T_b - T_{\infty}}{2T_b - (T_1 + T_{\infty})}$$

$$T^* = \frac{20,000}{24.2 - \ln(pX_{O_2})}$$

- $T^*$  is the midpoint of the NTC region obtained using the semi-empirical correlation (Seshadri et.al. (2015))
- $T^* = T_b$  and same for all three alkanes

# Liñán's Partial Burning Regime: Flame Standoff Ratio

$$\frac{r_b}{r_\ell} = \ln(1 + B) / \ln \left[ \frac{1 + B}{1 + c_p(T_b - T_\ell)/L} \right]$$



Farouk and Dryer (2014): n-heptane burning in air

## Liñán's Partial Burning Regime: Flame Standoff Ratio

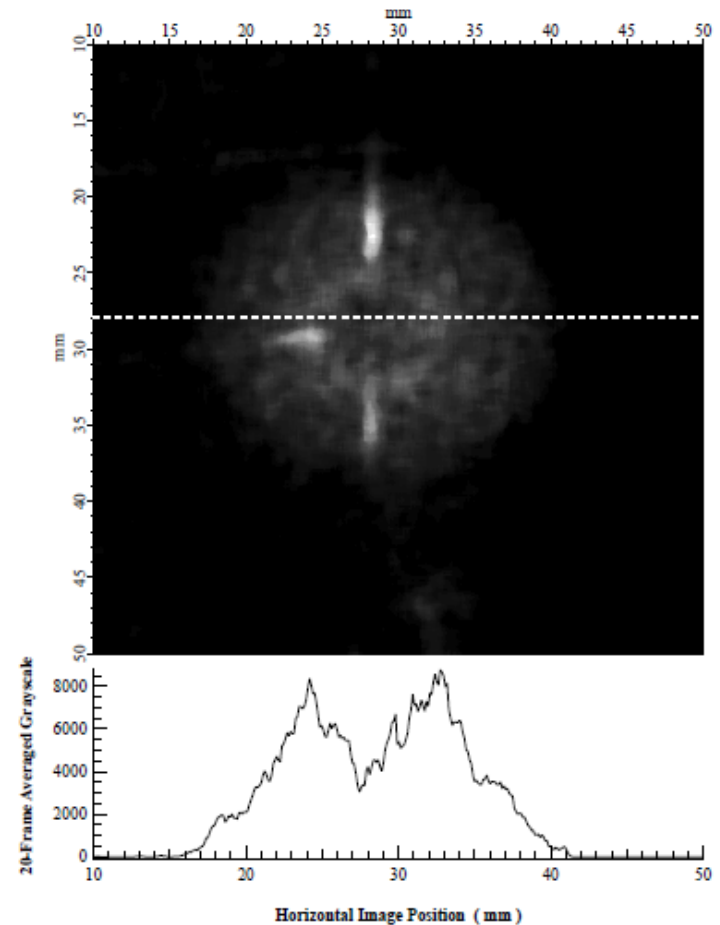
$$\frac{r_b}{r_\ell} = \ln(1 + B) / \ln \left[ \frac{1 + B}{1 + c_p(T_b - T_\ell)/L} \right]$$

- Farouk and Dryer FSR varies between 2.6 and 3.3. QS theory gives 3.1 in close agreement
- As observed by F&D no dependencies on  $D_0$  or  $\text{CO}_2$  concentration – only  $\text{O}_2$  concentration determines FSR
- Expression is very similar to the classical hot-flame FSR equation
- Hot flame FSR QS model predicts FSR orders of magnitude greater than experimental or numerical results
- Hot flames for n-alkanes lie in the outer transient-diffusive zone. Cool flames lie close to the droplet surface in the convective-diffusive zone where QS theories are applicable!
- Applies to all normal alkanes ( $T^*$  is very close to each other)
- Should be useful in planning CFI experiments

# Liñán's Partial Burning Regime: Flame Standoff Ratio

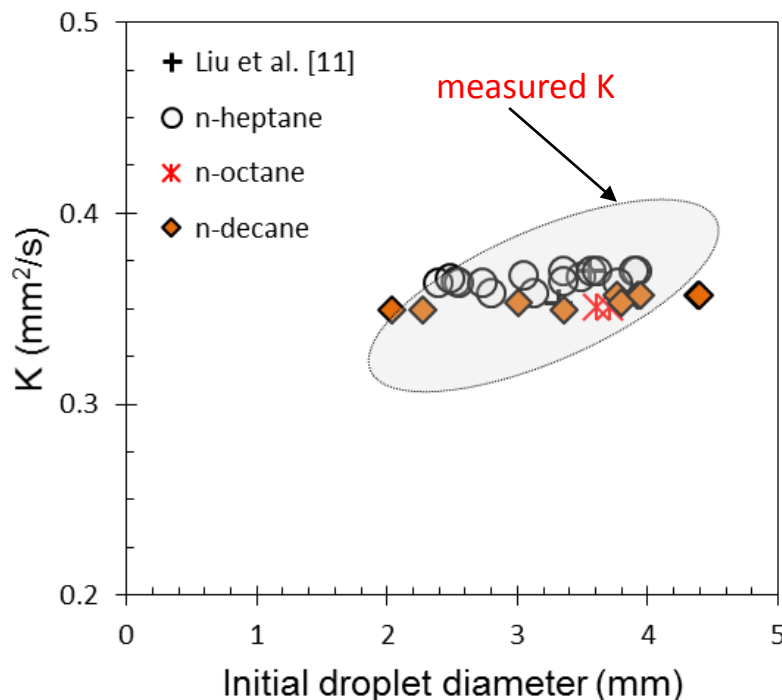
- QS cool flame visualized for the first time
- FLEX hardware changed – removed all spectral filters turned down the backlight
- N-Decane burning in air at 1 atm
- Image 10 to 20 frame averaged
- Measured FSR 3.2, predicted 3.1!

Experimental confirmation!



## Liñán's Partial Burning Regime: Burning Rate

$$K = \frac{8\lambda}{c_p \rho_\ell} \ln \left[ 1 + \frac{2T_b - (T_\ell + T_\infty)}{L/c_p} \right] = \frac{8\lambda}{c_p \rho_\ell} \ln(1 + B)$$



- Expression is very similar to the classical hot-flame burning rate constant equation
- Turn-over or NTC temperature rather than adiabatic flame temperature
- Predicts  $K$  within  $\pm 20\%$
- Applies to all normal alkanes ( $T^*$  is very close to each other)
- Shows there is a systematic dependence on initial droplet diameter and pressure
- Should be useful in planning CFI experiments

## Corrections to the Burning Rate: Oxygen Depletion Effect

- The initial hot flame depletes oxygen in the far field prior to cool flame start
- A correction to the oxygen concentration at the start of the cool flame can be estimated
- Hot flame is a sink for oxygen and convection is small far away from the droplet

$$\dot{m}_f = \frac{\pi}{4} \rho_\ell K_h D_s$$

$$\dot{m}_O = \nu \frac{\pi}{4} \rho_\ell K_h D_s$$

$$\frac{\partial Y}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 D \frac{\partial Y}{\partial r} \right)$$

$$t = 0 : Y = Y_{\infty,0} \quad (0 < r < \infty)$$

$$t > 0 : Y = Y_{\infty,0} \quad \text{as } r \rightarrow \infty$$

$$\lim_{r \rightarrow 0} \left( 4\pi r^2 \rho D \frac{\partial Y}{\partial r} \right) = \dot{m}_O \quad \text{as } r \rightarrow 0$$

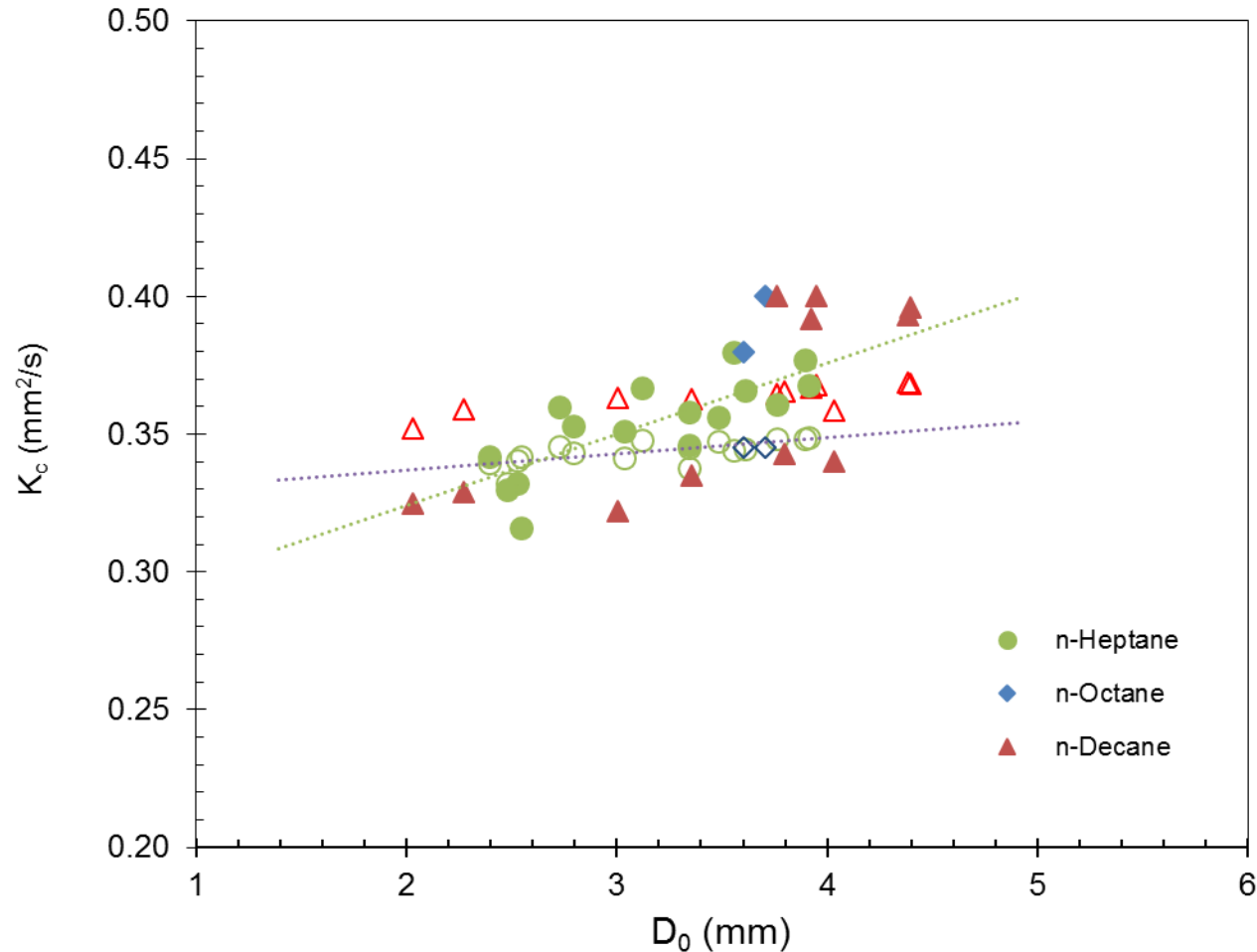
$$\dot{m}_O = \dot{M}_O f(t) = \frac{\pi}{4} \nu \rho_\ell K_h D_0 \sqrt{1 - K_h t / D_{s0}}$$

Using matched asymptotic technique the depleted oxygen concentration:

$$Y_r \sim Y_{\infty,0} - \frac{1}{32} \nu \left( \frac{K_h}{D_\infty} \right)^2 \frac{\rho_\ell}{\rho_\infty} \sqrt{\frac{D_\infty t_{he}}{\pi(D_0^2 - K_h t_{he})}}.$$

# Corrections to the Burning Rate: Oxygen Depletion Effect

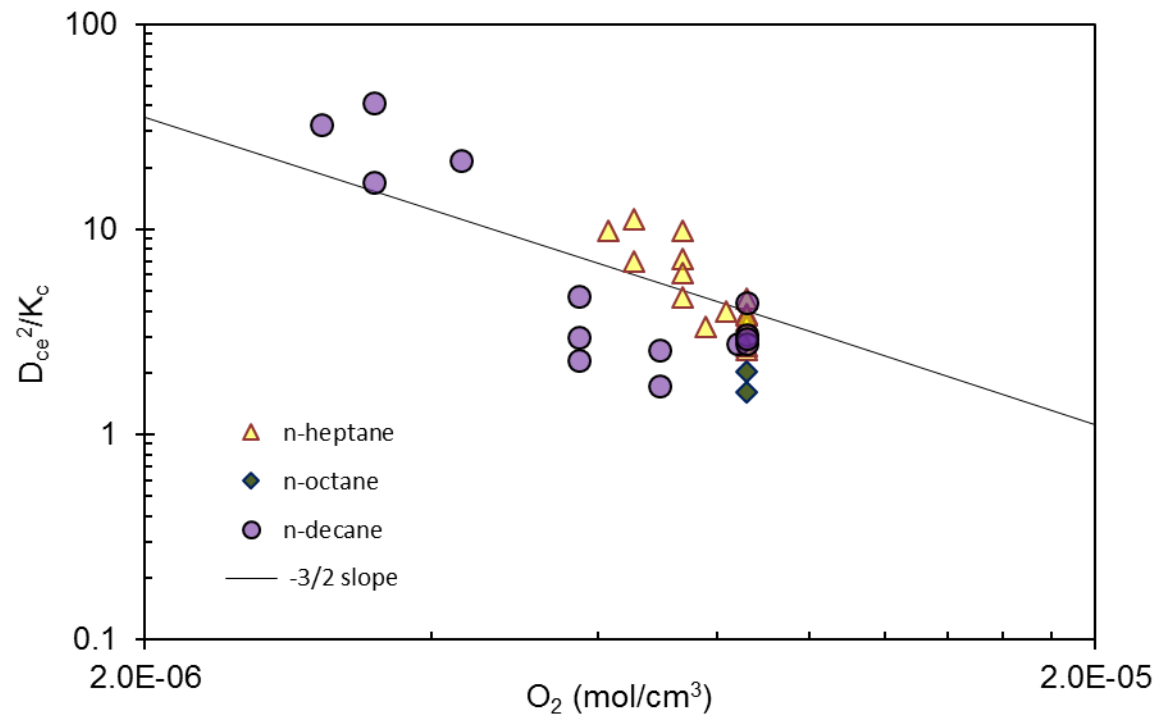
- Simple, approximate theory predicts the trend of increasing  $K_c$  with  $D_0$



- Improves the correlation a little – but still something is missing!

## Cool Flame Extinction

- Ketohydroperoxides decomposition chemical time:  $\tau = Ae^{180/RT}$
- Crossover temperature variation with Oxygen Concentration:  $C_{O_2} = Be^{-120/RT}$
- The chemical time becomes:  $\tau = AB^{3/2}/C_{O_2}^{3/2}$



- Residence time correlated against chemical time

## Concluding Remarks

- Cool flame burning rates and flame standoff ratios are reasonably well predicted using Liñán's partial burning regime
- Cool flame extinction diameters are correlated against  $C_{O_2}^{-3/2}$
- At higher pressures correlation does not work well
- Experiments indicate the pressure effects are not well captured by existing reduced mechanisms and needs further study
- Many aspects of the cool flame combustion still remains to be studied

## Related Publications

1. Nayagam, V., Dietrich, D. L., Ferkul, P. V., Hicks, M. C., and Williams, F. A. (2012). Can cool flames support quasi-steady alkane droplet burning? *Combustion and Flame*, 159(12), 3583-3588.
2. Nayagam, V., Dietrich, D.L., Hicks, M.C., and Williams, F.A., "Cool-flame extinction during n-alkane droplet combustion in microgravity." *Combustion and Flame*, Vol. 162, 2015, pp. 2140-2147.
3. Nayagam, V., Dietrich, D.L., and Williams, F.A., "Applications of the Partial-Burning Regime to Quasi-Steady n-Alkane Droplet Combustion Supported by Cool Flames," *AIAA Journal*, accepted, December 2015).
4. Paczko, G., Peters, N., Seshadri, K., and Williams, F.A., "The Role of Cool-Flame Chemistry in Quasi-Steady Combustion and Extinction of n-Heptane Droplets," *Combustion Theory and Modelling* 18.4-5 (2014): 515-531.
5. Seshadri, K., Peters, N., Williams, F.A., and Nayagam, V., "Asymptotic Analysis of Quasi-Steady Heptane Droplet Combustion Supported by Cool-Flame Chemistry," *Combustion Theory and Modelling*, (submitted, February 2015)

# Flame Extinguishment Experiment (FLEX) Science Team

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Questions?

